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COMPUTED HEATS OF FORMATION OF THREE TETRAAZAPENTALENES, A TRIS(NITROTRIAZOLO)TRIAZINE, AND A TRICYCLIC *GEM*-DIFLUORAMINO/TETRANITRAMINE

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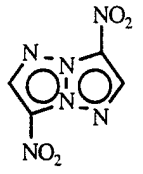
13. ABSTRACT *(Maximum 200 words)*

Computed heats of formation for **1** - **5**.



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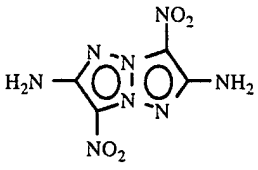

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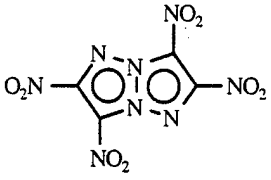

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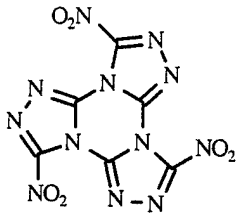

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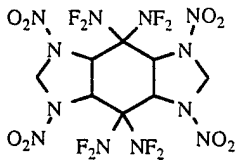

5

1: ΔH_f^{298K} (solid) = 114 kcal/mole = 573 cal/g

2: ΔH_f^{298K} (solid) = 91 kcal/mole = 400 cal/g

3: ΔH_f^{298K} (solid) = 141 kcal/mole = 489 cal/g

4: ΔH_f^{298K} (solid) = 225 kcal/mole = 668 cal/g

5: ΔH_f^{298K} (solid) = 9 kcal/mole = 16 cal/g

14. SUBJECT TERMS
heats of formation; tetraazapentalenes; tris(nitrotriazolo)-triazine; tricyclic gem-difluoramino/tetranitramine

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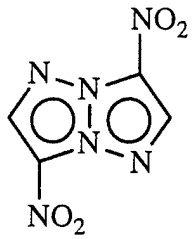
We have used our density functional procedure [1] to compute the heats of formation of the compounds **1** - **5**, proposed by W. Koppes and A. Stern (ONR). The vibrational energies were determined from the molecular stoichiometries [2]. The density functional calculations give the gas phase heat of formation, which we convert to the solid state value by subtracting the heat of sublimation. The latter is obtained by means of the relationship that we have developed between the heat of sublimation and the computed electrostatic potential on the molecular surface [3].

Results:

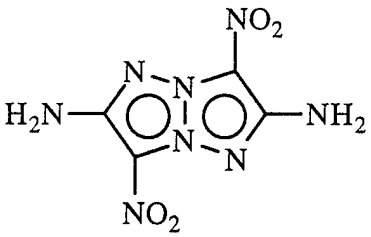
1



ΔH_f^{298K} (gas) = 138 kcal/mole = 694 cal/g

ΔH_f^{298K} (solid) = 114 kcal/mole = 573 cal/g

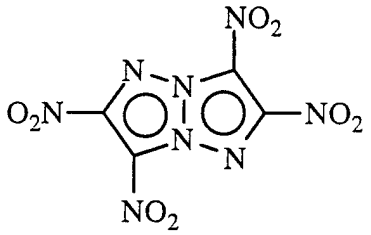
2



ΔH_f^{298K} (gas) = 120 kcal/mole = 526 cal/g

ΔH_f^{298K} (solid) = 91 kcal/mole = 400 cal/g

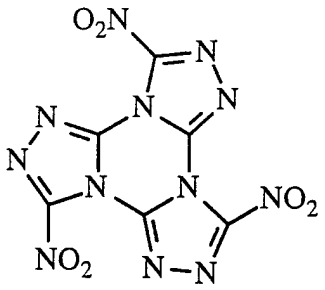
3



ΔH_f^{298K} (gas) = 172 kcal/mole = 597 cal/g

ΔH_f^{298K} (solid) = 141 kcal/mole = 489 cal/g

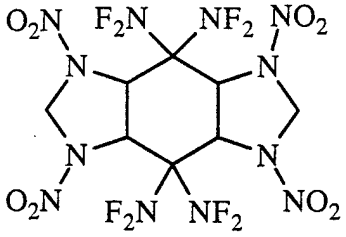
4



ΔH_f^{298K} (gas) = 266 kcal/mole = 790 cal/g

ΔH_f^{298K} (solid) = 225 kcal/mole = 668 cal/g

5



ΔH_f^{298K} (gas) = 63 kcal/mole = 114 cal/g

ΔH_f^{298K} (solid) = 9 kcal/mole = 16 cal/g

For comparison, the experimental gas phase ΔH_f^{298K} value for RDX is 206 cal/g [4,5].

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